

Ocimene (E)
3779-61-1 | DTXSID8040567

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 175 °C

Global applicability domain: Inside

Local applicability domain index: 8.23e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Myrcene</div> <div>Measured: 167</div> <div>Predicted: 172</div>	<div>Image not found</div> <div>2,6-Dimethyl-2,4,6-octatriene</div> <div>Measured: 188</div> <div>Predicted: 180</div>	<div>Image not found</div> <div>3-Methylidene-6-(propan-2-yl)cyclohexene</div> <div>Measured: 172</div> <div>Predicted: 173</div>
<div>Image not found</div> <div>alpha-Phellandrene</div> <div>Measured: 172</div> <div>Predicted: 174</div>	<div>Image not found</div> <div>alpha-Terpinene</div> <div>Measured: 175</div> <div>Predicted: 177</div>	